Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:

Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations

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Table S1: Calculated (B3LYP/def2-SVP) ^{13}C chemical shift (ppm) for model H. Results for equivalent nuclei are given in groups. The numbering of groups and nuclei refers to Figure 10.

Group/Nucleus	$\delta_{in\ vacuo}$ [a]	δ_{sol} [b]	δ_a [c]	$\delta_{sol} - \delta_a$ [d]	$\delta_{sol} - \delta_{in\ vacuo}$ [e]
C3	131.74	125.66	-0.89	126.55	-6.08
C8	132.79	127.28	-0.86	128.14	-5.51
C14	138.24	132.75	-0.89	133.64	-5.49
C4	138.21	133.24	-0.93	134.17	-4.97
G3	142.80	139.63	-0.90	140.54	-3.17
G5	134.89	132.00	-0.89	132.88	-2.89
G2	122.25	124.33	-0.95	125.28	2.09
G9	161.34	164.28	-0.95	165.23	2.94
G7	128.81	134.27	-0.98	135.25	5.47
G8	134.17	139.69	-0.95	140.64	5.51
G4	136.20	141.80	-1.00	142.80	5.60
G1	122.19	128.55	-1.00	129.54	6.35
G6	126.93	133.74	-0.96	134.70	6.80

[a] *In vacuo* result.
[b] Dynamically solvated model.
[c] A posteriori extracted solvent magnetisability anisotropy correction.
[d] Approximate electrostatic contribution, δ_E.
[e] Total solvation-induced change.

Table S2: Calculated (B3LYP/def2-SVP) ^{13}C chemical shift (ppm) for model G. Results for equivalent nuclei are given in groups. The numbering of groups and nuclei refers to Figure 10.

Group/Nucleus[a]	$\delta_{in\ vacuo}$[b]	δ_{sol}[c]	δ_a[d]	$\delta_{sol} - \delta_a$[e]	$\delta_{sol} - \delta_{in\ vacuo}$[f]
C11	131.11	125.50	-0.94	126.44	-5.60
C6	134.44	129.00	-0.90	129.90	-5.44
C14	138.29	133.65	-0.97	134.62	-4.64
C13	135.46	132.23	-0.93	133.16	-3.23
C10	143.02	139.98	-0.95	140.93	-3.04
C12	143.03	140.45	-0.95	141.40	-2.57
C7	128.37	128.13	-0.94	129.07	-0.24
C5	132.92	132.82	-0.91	133.73	-0.09
C4	156.18	157.57	-0.92	158.48	1.39
G3	121.12	123.55	-0.99	124.54	2.43
G2	161.49	164.41	-0.99	165.40	2.92
G1	48.06	51.82	-1.04	52.86	3.76
C24	130.35	134.75	-0.97	135.73	4.40
C19	135.94	140.94	-1.04	141.98	5.00
C18	121.59	127.01	-1.03	128.05	5.42
C16	136.19	141.94	-1.05	142.98	5.74
C17	120.41	127.16	-1.04	128.20	6.75
C26	127.19	134.00	-1.00	135.00	6.81
C25	127.14	134.39	-1.02	135.41	7.25
C8	127.91	135.65	-1.02	136.67	7.74
C9	118.45	137.80	-1.00	138.80	19.35

[a] The practically chemically equivalent nuclei that are averaged over, are C21-C23.
[b] *In vacuo* result.
[c] Dynamically solvated model.
[d] A posteriori extracted solvent magnetisability anisotropy correction.
[e] Approximate electrostatic contribution, δ_E.
[f] Total solvation-induced change.

Table S3: Calculated (B3LYP/def2-SVP) ^{13}C chemical shift (ppm) for model F. Results for equivalent nuclei are given in groups. The numbering of groups and nuclei refers to Figure 10.

Group/Nucleus[a]	$\delta_{in\ vacuo}$[b]	δ_{sol}[c]	δ_a[d]	$\delta_{sol} - \delta_a$[e]	$\delta_{sol} - \delta_{in\ vacuo}$[f]
C21	131.32	125.20	-0.95	126.15	-6.12
C16	134.87	130.05	-0.92	130.97	-4.82
C24	138.07	133.36	-0.97	134.34	-4.70
C22	142.94	139.09	-0.97	140.05	-3.85
C20	142.57	138.95	-0.98	139.93	-3.61
C14	152.29	149.35	-0.88	150.23	-2.94
C23	135.32	132.79	-0.96	133.75	-2.53
C15	135.83	133.33	-0.90	134.22	-2.51
G1	151.83	149.64	-0.87	150.51	-2.19
C17	131.36	130.62	-0.96	131.59	-0.73
G4	126.60	128.32	-0.95	129.27	1.72
C34	131.95	133.95	-0.96	134.91	2.00
G6	121.53	123.76	-0.99	124.75	2.23
G2	124.89	127.13	-1.00	128.13	2.24
G5	161.40	164.44	-0.98	165.41	3.04
G3	131.21	134.68	-1.00	135.68	3.47
C26	136.12	141.11	-1.06	142.17	4.99
C36	126.99	132.87	-1.04	133.91	5.88
C35	127.91	134.35	-1.05	135.41	6.44
C29	135.96	142.73	-1.06	143.79	6.77
C28	121.83	128.85	-1.06	129.91	7.02
C18	127.46	134.54	-1.04	135.58	7.08
C27	121.40	128.70	-1.07	129.77	7.29
C19	130.73	141.26	-0.98	142.25	10.54

[a] The practically chemically equivalent nuclei that are averaged over, are C30-C25 and C31-C33.
[b] *In vacuo* result.
[c] Dynamically solvated model.
[d] A posteriori extracted solvent magnetisability anisotropy correction.
[e] Approximate electrostatic contribution, δ_E.
[f] Total solvation-induced change.

Table S4: Calculated (B3LYP/def2-SVP) ^{13}C chemical shift (ppm) for model E. Results for equivalent nuclei are given in groups. The numbering of groups and nuclei refers to Figure 11.

Group/Nucleus	$\delta_{in\ vacuo}$ [a]	δ_{sol} [b]	δ_a [c]	$\delta_{sol} - \delta_a$ [d]	$\delta_{sol} - \delta_{in\ vacuo}$ [e]
C8	134.21	127.78	-0.88	128.66	-6.43
C14	135.82	130.82	-0.92	131.75	-5.00
G1	146.83	141.94	-0.91	142.85	-4.89
G2	133.05	128.38	-0.88	129.26	-4.67
C3	134.25	129.71	-0.91	130.62	-4.54
C4	129.92	131.53	-0.97	132.50	1.61
G10	161.99	164.12	-0.99	165.11	2.13
G4	120.42	122.72	-0.98	123.70	2.30
G3	139.12	143.47	-0.89	144.36	4.35
G9	26.68	31.11	-1.03	32.14	4.43
G5	127.13	132.76	-1.00	133.75	5.63
G6	131.72	138.19	-0.94	139.13	6.47
G7	132.61	141.76	-0.99	142.75	9.14
G8	131.76	148.08	-0.96	149.03	16.31

[a] *In vacuo* result.
[b] Dynamically solvated model.
[c] A posteriori extracted solvent magnetisability anisotropy correction.
[d] Approximate electrostatic contribution, δ_E.
[e] Total solvation-induced change.

Table S5: Calculated (B3LYP/def2-SVP) ^{13}C chemical shift (ppm) for model D. Results for equivalent nuclei are given in groups. The numbering of groups and nuclei refers to Figure 11.

Group/Nucleus	$\delta_{in\ vacuo}$ [a]	δ_{sol} [b]	δ_a [c]	$\delta_{sol} - \delta_a$ [d]	$\delta_{sol} - \delta_{in\ vacuo}$ [e]
G1	147.62	141.00	-0.93	141.93	-6.62
C8	133.90	128.32	-0.89	129.22	-5.58
C14	135.54	130.92	-0.95	131.87	-4.63
G2	132.69	128.35	-0.90	129.25	-4.34
C3	133.63	129.78	-0.93	130.72	-3.84
G3	137.24	134.79	-0.98	135.77	-2.46
G5	131.29	132.89	-1.03	133.91	1.60
C4	130.58	132.38	-1.00	133.38	1.80
G9	142.13	144.18	-0.91	145.09	2.05
G7	120.29	122.69	-1.02	123.72	2.40
G6	161.40	164.34	-1.05	165.38	2.94
G10	131.22	134.27	-1.03	135.30	3.05
G4	139.31	143.59	-0.91	144.49	4.28
G13	127.18	132.51	-1.04	133.55	5.33
G12	132.90	139.74	-0.97	140.72	6.85
G11	132.66	142.07	-1.02	143.10	9.41
G8	137.25	148.77	-0.99	149.76	11.53

[a] *In vacuo* result.
[b] Dynamically solvated model.
[c] A posteriori extracted solvent magnetisability anisotropy correction.
[d] Approximate electrostatic contribution, δ_E.
[e] Total solvation-induced change.

Table S6: Calculated (B3LYP/def2-SVP) ^{13}C chemical shift (ppm) for model C. Results for equivalent nuclei are given in groups. The numbering of groups and nuclei refers to Figure 11.

Group/Nucleus[a]	$\delta_{in\ vacuo}$[b]	δ_{sol}[c]	δ_a[d]	$\delta_{sol} - \delta_a$[e]	$\delta_{sol} - \delta_{in\ vacuo}$[f]
C11	136.38	131.30	-0.89	132.19	-5.08
C13	145.47	140.66	-0.94	141.60	-4.81
C5	133.25	128.52	-0.94	129.46	-4.73
C10	133.27	129.06	-0.90	129.96	-4.21
C3	144.28	140.40	-0.94	141.34	-3.88
C12	127.23	124.90	-0.91	125.80	-2.33
C19	130.75	130.77	-0.90	131.67	0.02
G3	162.05	163.39	-1.03	164.43	1.35
C6	130.13	131.62	-1.00	132.61	1.49
C15	120.19	122.72	-1.01	123.73	2.53
C4	139.54	142.82	-0.92	143.74	3.28
C7	118.92	122.56	-1.02	123.58	3.64
G2	26.83	31.22	-1.05	32.27	4.38
C9	139.24	143.78	-0.92	144.70	4.53
G1	48.40	53.19	-1.03	54.22	4.79
C20	155.01	160.02	-0.91	160.93	5.01
C22	133.35	139.14	-0.96	140.10	5.79
C23	129.23	136.03	-0.97	137.01	6.80
C24	125.27	132.22	-1.02	133.24	6.95
C25	131.57	138.77	-0.96	139.73	7.19
C8	132.02	148.37	-1.00	149.37	16.36
C14	131.45	148.30	-0.99	149.29	16.86
C21	117.28	134.31	-0.97	135.27	17.03

[a] The practically chemically equivalent nuclei that are averaged over, are C1-C27 and C16-C18.
[b] *In vacuo* result.
[c] Dynamically solvated model.
[d] A posteriori extracted solvent magnetisability anisotropy correction.
[e] Approximate electrostatic contribution, δ_E.
[f] Total solvation-induced change.

Table S7: Calculated (B3LYP/def2-SVP) ^{13}C chemical shift (ppm) for model B. Results for equivalent nuclei are given in groups. The numbering of groups and nuclei refers to Figure 12.

Group/Nucleus[a]	$\delta_{in\ vacuo}$[b]	δ_{sol}[c]	δ_a[d]	$\delta_{sol} - \delta_a$[e]	$\delta_{sol} - \delta_{in\ vacuo}$[f]
C18	149.63	140.87	-0.97	141.84	-8.76
C16	137.94	131.13	-0.93	132.06	-6.81
C8	148.86	142.19	-0.97	143.16	-6.67
G3	140.67	134.18	-1.01	135.19	-6.49
C15	134.77	128.90	-0.95	129.85	-5.87
C10	134.87	129.61	-0.98	130.59	-5.26
G2	140.39	135.18	-1.02	136.20	-5.21
C24	135.41	130.38	-0.92	131.30	-5.03
G6	153.79	149.05	-0.91	149.96	-4.74
C17	131.59	127.83	-0.94	128.77	-3.75
C25	152.30	150.56	-0.90	151.46	-1.74
C2	144.42	142.84	-0.96	143.80	-1.58
G7	129.63	128.32	-0.98	129.30	-1.30
G5	134.16	133.59	-1.05	134.63	-0.57
G4	134.07	133.82	-1.07	134.89	-0.25
C11	132.43	132.21	-1.04	133.25	-0.22
G9	127.51	127.69	-1.03	128.72	0.17
G8	133.98	134.60	-1.04	135.64	0.62
C32	143.99	144.91	-0.95	145.87	0.92
C12	121.63	122.78	-1.06	123.84	1.15
C20	122.16	123.31	-1.06	124.37	1.15
C9	140.86	142.28	-0.95	143.24	1.42
C28	133.74	136.29	-1.00	137.29	2.55
C14	141.11	143.79	-0.96	144.74	2.68
G1	161.44	164.16	-1.08	165.24	2.73
C29	129.16	132.23	-1.09	133.32	3.07
C27	136.89	140.35	-1.01	141.36	3.46
C30	135.75	139.96	-1.03	140.99	4.21
C26	132.80	138.03	-1.00	139.03	5.24
C19	139.73	148.76	-1.02	149.78	9.03
C13	140.26	149.37	-1.04	150.41	9.11

[a] The practically chemically equivalent nuclei that are averaged over, are C1-C3, C21-C23, C33-C37, C4-C5-C6 and C34-C35-C36.
[b] *In vacuo* result.
[c] Dynamically solvated model.
[d] A posteriori extracted solvent magnetisability anisotropy correction.
[e] Approximate electrostatic contribution, δ_E.
[f] Total solvation-induced change.

Table S8: Calculated (B3LYP/def2-SVP) ^{13}C chemical shift (ppm) for model A. Results for equivalent nuclei are given in groups. The numbering of groups and nuclei refers to Figure 12.

Group/Nucleus[a]	$\delta_{in\ vacuo}$[b]	δ_{sol}[c]	δ_a[d]	$\delta_{sol} - \delta_a$[e]	$\delta_{sol} - \delta_{in\ vacuo}$[f]
C16	136.08	130.58	-0.97	131.55	-5.50
C8	145.46	140.26	-0.99	141.25	-5.20
C10	132.89	127.76	-1.02	128.78	-5.13
C18	146.31	141.49	-1.01	142.50	-4.82
G6	150.00	145.63	-0.93	146.56	-4.38
C15	132.74	128.87	-1.01	129.87	-3.88
C24	132.96	129.82	-0.94	130.77	-3.13
C17	128.89	125.79	-0.98	126.76	-3.11
G3	136.67	133.80	-1.06	134.85	-2.87
G2	136.48	133.82	-1.05	134.87	-2.66
C25	151.57	150.11	-0.93	151.04	-1.46
C2	143.35	142.30	-1.00	143.30	-1.05
C32	143.06	142.89	-1.01	143.90	-0.17
C11	130.91	131.03	-1.07	132.10	0.13
G9	150.40	150.75	-0.92	151.68	0.35
C14	140.04	140.63	-1.01	141.64	0.59
G7	126.60	127.30	-0.99	128.29	0.70
G1	161.25	162.07	-1.10	163.17	0.82
G13	37.65	38.69	-0.99	39.67	1.04
G12	60.66	61.92	-0.93	62.85	1.26
G11	37.01	38.38	-1.00	39.38	1.37
G4	130.86	132.70	-1.11	133.81	1.84
G5	130.91	132.84	-1.08	133.92	1.93
C12	119.39	121.45	-1.08	122.53	2.06
G8	129.37	132.03	-1.00	133.02	2.66
G10	45.41	48.08	-0.91	48.99	2.66
C20	120.13	123.03	-1.09	124.12	2.90
G14	38.28	41.27	-0.91	42.18	2.99
C9	139.69	142.70	-0.99	143.69	3.01
C30	133.03	136.28	-1.08	137.36	3.26
C28	131.04	136.01	-1.01	137.01	4.96
C29	125.67	131.14	-1.11	132.25	5.47
C27	134.36	139.99	-1.03	141.01	5.62
C26	128.59	137.68	-1.02	138.69	9.09
C13	137.99	148.36	-1.04	149.40	10.37
C19	137.45	148.16	-1.06	149.22	10.71

[a] See the footnote *a* in Table S7.
[b] *In vacuo* result.
[c] Dynamically solvated model.
[d] A posteriori extracted solvent magnetisability anisotropy correction.
[e] Approximate electrostatic contribution, δ_E.
[f] Total solvation-induced change.

Table S9: Calculated (def2-SVP) ^{13}C chemical shifts (ppm) for perylene with different methods in the *in vacuo* model. Results are given for groups of equivalent nuclei. The reference (CH_4) shielding constants are (in ppm): $\sigma_{ref} = 201.32, 198.39, 195.62$ and 193.03, with HF, BHandHLYP, B3LYP and BLYP, respectively.

Group[a]	HF	BHandHLYP	B3LYP	BLYP
G1	138.72	140.04	138.87	137.33
G2	133.30	134.66	133.45	131.90
G3	136.05	137.84	136.98	135.56
G4	130.79	131.72	130.48	128.75
G5	123.63	124.20	122.74	120.86
G6	129.11	129.61	128.20	126.38

[a] See Figure 5 of the main article.

Table S 10: Calculated ^{13}C chemical shift (ppm) for model B with different basis sets and shell thicknesses at the B3LYP level. Results for equivalent nuclei are given in groups. $\sigma_{\text{ref}} = 195.62$ and 190.30 ppm with def2-SVP and def2-TZVP, respectively.

Shell thickness	*In vacuo*		3.5 Å		5 Å
Group*	def2-SVP	def2-TZVP	def2-SVP	def2-TZVP	def2-SVP
G1	140.39	148.8	138.53	150.41	138.34
C2	144.42	155.53	151.36	163.01	151.10
G3	134.07	140.52	132.50	142.45	132.80
C8	148.86	156.26	148.74	160.14	148.79
C9	140.86	149.77	145.07	156.80	145.62
C10	134.87	143.13	130.64	141.75	130.34
C11	132.43	140.29	128.91	138.64	128.85
C12	121.63	128.61	119.73	128.85	119.02
C13	140.26	147.20	147.31	154.05	147.55
C14	141.11	150.13	137.34	146.31	138.02
C15	134.77	143.15	124.79	134.70	124.32
C16	137.94	146.93	127.82	139.33	127.80
C17	131.59	139.48	133.24	144.31	132.46
C18	149.63	157.37	138.30	148.14	136.98
C19	139.73	146.24	148.52	158.07	148.20
C20	122.16	129.21	129.43	138.03	128.76
C21	161.50	172.97	166.89	175.17	166.95
C23	161.37	172.65	166.56	176.93	166.58
C24	135.41	143.61	133.51	145.22	133.80
C25	152.30	162.72	141.14	152.33	142.71
C26	132.80	138.32	130.28	139.36	130.87
C27	136.89	144.77	140.86	145.15	141.88
C28	133.74	139.81	136.54	145.26	138.13
C29	129.16	135.05	127.09	139.69	127.17
C30	135.75	143.32	138.11	150.82	138.43
C32	143.99	155.05	148.86	162.12	149.27
G2	140.67	149.07	136.06	149.56	136.04
G4	134.16	140.69	133.53	142.31	133.26
G5	153.79	166.60	149.97	164.29	149.63
G6	129.63	137.34	126.73	137.66	126.72
G7	133.98	140.91	131.23	141.77	131.64
G8	127.51	133.28	126.68	135.36	127.76

$*$ See Fig. 12 of the main article.

Table S 11: Calculated first four and five singlet excited state energies in each of the relevant irreps of perylene up to $-e(\mathrm{HOMO})$ 5.11 eV and acetonitrile *in vacuo*. The magnetically allowed excited states and corresponding irreps at which the magnetic transition dipole moment operates in, are given.

System	Perylene			CH_3CN	
Point group	State	Energy (eV)	Point group	State	Energy (eV)
D_{2h}	$1B_{1g}$	3.69	C_{3v}	$1A_2$	7.95
	$2B_{1g}$	4.03		$2A_2$	11.26
	$3B_{1g}$	4.12		$3A_2$	12.23
	$4B_{1g}$	4.62		$4A_2$	14.64
	$1B_{2g}$	5.79		1E	8.25
	$2B_{2g}$	6.44		2E	9.29
	$3B_{2g}$	7.27		3E	9.42
	$4B_{2g}$	7.60		4E	11.33
	$5B_{2g}$	7.62		5E	12.22
	$1B_{3g}$	5.77			
	$2B_{3g}$	6.46			
	$3B_{3g}$	7.61			
	$4B_{3g}$	7.63			
	$5B_{3g}$	7.93			

Table S 12: The calculated singlet excited state energies up to $-e(\mathrm{HOMO})$ values 5.51, 5.67 and 5.43 eV of perylene. The perylene molecule was dissolved in acetonitrile in the MD snapshot numbers 103, 457 and 735.

	Snapshot number		
State	103	457	735
A1	2.62	2.46	2.56
A2	3.56	3.38	3.48
A3	3.86	3.58	3.67
A4	3.94	3.72	3.83
A5	4.03	3.98	3.93
A6	4.19	4.01	4.02
A7	4.39	4.32	4.07
A8	4.47	4.36	4.21
A9	4.48	4.69	4.32
A10	4.73	4.85	4.36
A11	4.81	4.95	4.37
A12	4.97	4.96	4.43
A13	5.12	4.98	4.56
A14	5.23	5.00	4.62
A15	5.25	5.09	4.68
A16	5.28	5.17	4.70
A17	5.31	5.20	4.74
A18	5.33	5.24	4.87
A19	5.36	5.25	4.88
A20	5.40	5.27	4.94
A21	5.41	5.29	4.99
A22	5.43	5.29	5.03
A23	5.44	5.33	5.04
A24	5.46	5.35	5.15
A25	5.47	5.39	5.15
A26	5.48	5.41	5.22
A27	5.51	5.42	5.25
A28	-	5.47	5.26
A29	-	5.47	5.31
A30	-	5.49	5.33
A31	-	5.52	5.35
A32	-	5.54	5.40
A33	-	5.55	5.43
A34	-	5.58	5.43
A35	-	5.59	-
A36	-	5.60	-
A37	-	5.62	-
A38	-	5.63	-
A39	-	5.64	-
A40	-	5.67	-
A41	-	5.67	-
A42	-	-	-

Table S 13: XYZ coordinates of the perylene snapshots 103, 457 and 735.

103

134

C	10.343996	13.304076	2.937743
C	10.212652	14.567998	3.166491
C	9.183296	15.079359	3.953799
C	8.331635	14.183509	4.663478
C	8.591151	12.865922	4.59111
C	9.620253	12.387462	3.753271
C	9.018496	16.436913	4.173561
C	8.038981	16.992094	4.963413
C	7.148529	16.091385	5.520352
C	7.308627	14.725094	5.433372
C	7.803821	12.001899	5.366462
C	6.744271	12.481566	6.176069
C	6.487098	13.886533	6.28135
C	7.995658	10.597014	5.271635
C	7.327615	9.738151	6.123867
C	6.362014	10.196754	6.964258
C	6.048182	11.568151	6.988921
C	5.055135	12.033624	7.820213
C	4.838907	13.385682	7.959556
C	5.567928	14.291003	7.255911
H	11.041883	12.937104	2.154213
H	10.811128	15.271206	2.611541
H	9.823648	11.341228	3.587617
H	9.731119	17.13747	3.815348
H	8.036787	18.094229	5.060575
H	6.347365	16.554386	6.100068
H	8.727252	10.148416	4.658556
H	7.542068	8.675117	6.123105
H	5.880305	9.51864	7.551737
H	4.487565	11.271161	8.350753
H	4.105225	13.761704	8.670495
H	5.419284	15.336977	7.411496
N	5.877815	17.3892244963	9.373132
C	4.843522	17.8632634963	9.419606
C	3.554116	18.4111684963	9.515473
H	3.632723	19.5270864963	9.365111
H	2.98941	17.8271824963	8.777675
H	3.077389	18.1393934963	10.496287
N	11.161181	11.352696	7.289963
C	11.179927	12.444489	6.975836
C	11.351716	13.866418	6.674842
H	10.551435	14.422042	7.132419
H	12.27057	14.093701	7.168747
H	11.310433	14.032941	5.634222
N	7.49795	9.914169	11.439813
C	7.892166	10.50659	10.563367
C	8.480301	11.253931	9.471613
H	7.873742	12.110425	9.213592
H	9.515787	11.488688	9.593423
H	8.546343	10.552282	8.698494
N	9.328139	20.2220714963	6.449235
C	9.230817	19.4085464963	7.267931
C	8.977	18.2981764963	8.162595
H	8.733851	17.4392574963	7.484399
H	9.890271	17.9911174963	8.651271
H	8.228551	18.5150134963	8.874974
N	8.752032	4.63945	4.957269
C	8.405002	5.078071	5.984347
C	7.817941	5.601124	7.245683
H	6.735334	5.355962	7.343261
H	8.344063	5.17069	8.011974
H	7.973019	6.673165	7.156926
N	11.771442	20.3006044963	1.176565
C	11.075338	20.4798124963	2.074514
C	10.175356	20.6685984963	3.263883
H	9.304156	21.1893944963	2.891609
H	9.941664	19.7133084963	3.688791
H	10.753247	21.2964034963	3.97311
N	2.652808	15.9388544963	14.585591
C	2.73059	15.6494464963	13.474185
C	2.899295	15.2537194963	12.088218
H	2.002428	15.5022004963	11.563525
H	3.733877	15.7791814963	11.644717
H	3.22231	14.1723094963	12.019032
N	11.58451	9.916203	-1.771686
C	12.057681	10.672658	-1.028203
C	12.741393	11.528929	-0.078928
H	13.61667	11.926054	-0.543813
H	12.105145	12.355278	0.214345
H	13.044271	10.940853	0.750987
N	13.593002	14.306174	2.416659
C	14.52344	13.639624	2.638354
C	15.685086	12.810344	2.9156
H	15.444785	11.827555	2.513309
H	16.551958	13.250779	2.406765
H	15.955812	12.759924	3.904872
N	10.561117	7.227619	6.575247
C	10.604536	7.57019	7.653711
C	10.510546	7.942345	9.045664
H	11.363894	7.657455	9.678347
H	10.552575	9.065957	9.024831
H	9.701109	7.511295	9.608452
N	8.268021	18.0513974963	0.905419
C	7.440957	17.3829824963	1.393945
C	6.401022	16.6404424963	2.042424
H	5.789222	16.3848044963	1.249382
H	6.658437	15.7880794963	2.680753
H	5.856823	17.3226094963	2.687865
N	5.211216	19.9406294963	6.054376
C	4.504731	19.1603024963	5.554058
C	3.679923	18.0236984963	4.963479
H	2.621641	18.2875744963	4.85502
H	4.079754	17.8540544963	3.914063

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N    2.280365  15.755531  7.115037
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C    1.304332  13.363009  7.518739
H    1.288932  13.092422  8.608253
H    0.2795  13.365509  7.223755
H    1.85242  12.653913  6.881091
N    9.519547  7.856456  2.35111
C    8.429414  7.669188  2.508854
C    7.026212  7.460591  2.785695
H    6.533998  8.21021  3.492597
H    6.41093  7.381113  1.933263
H    7.063406  6.625181  3.452178
N    3.517269  11.41848  4.250638
C    3.574716  12.542497  4.037503
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H    4.696079  14.356836  3.711709
H    3.186172  14.291165  2.915617
H    3.127126  14.605399  4.604135
N    11.00519  14.8205894963  -0.331913
C    11.471809  15.7537494963  0.050161
C    11.853048  17.0765404963  0.498747
H    10.930672  17.5138234963  0.833408
H    12.638962  17.0032874963  1.250925
H    12.170034  17.5758794963  -0.407211
N    5.99788  13.4047  1.569916
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C    6.818122  10.946772  1.865277
H    7.862355  10.800981  1.621693
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H    6.30127  10.29191  1.157101

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134

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C    -5.021798  -15.267385  2.72016
C    -5.101008  -13.898641  2.543061
C    -6.273434  -13.356435  2.000879
C    -7.32048  -14.20334  1.717125
C    -3.844109  -15.853327  3.149082
C    -2.755794  -15.022153  3.512316
C    -2.881486  -13.649491  3.487137
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C    -6.334879  -11.970702  1.879532
C    -5.290902  -11.07202  2.32214
C    -4.131208  -11.610235  2.924733
C    -7.443559  -11.250821  1.328206
C    -7.5938  -9.84313  1.262854
C    -6.558999  -9.021121  1.792247
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H    -7.972816  -16.234123  1.499008
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H    -8.293665  -13.81323  1.307161
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H    -2.04379  -13.12682  3.73382
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H    -8.498206  -9.410636  0.898479
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N    0.396888  -13.179873  1.425184
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H    -1.321374  -11.358337  -0.303917
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C    -1.684595  -20.5346636427  5.584982
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H    -2.667064  -20.6966316427  5.952204
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H    -8.170387  -20.0329886427  1.510249
H    -7.088418  -19.1007716427  2.439739
H    -8.118717  -20.2860846427  3.253294
N    -10.293106  -6.006068  2.372865
C    -9.694374  -6.144475  1.401388
C    -8.990387  -6.195294  0.166663
H    -7.932408  -5.893271  0.196724
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H    -9.549824  -5.592717  -0.513278
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C    -8.420738  -12.61771  5.288393
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H    -9.864361  -11.105636  4.820417
N    -6.587184  -7.627  -1.850999
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C    -5.645625  -9.988186  -1.516693
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H    -6.463911  -10.720047  -1.538427
H    -4.950503  -9.957584  -2.328605
N    2.139222  -17.5802066427  5.260287
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C    1.328669  -15.8678046427  3.452783
H    2.172491  -15.5866306427  2.766795
H    0.396614  -16.1461076427  2.932554
H    1.214716  -14.9122096427  3.988627
N    -3.279274  -15.729124  6.923087
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C    -11.670729  -18.6935296427  0.195426
C    -11.895643  -17.2657166427  0.176726
H    -12.212616  -16.8995056427  -0.828774
H    -12.759642  -16.9976606427  0.916198
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N    -5.073002  -19.2329676427  5.167594
C    -5.648044  -18.3372576427  5.541296
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N    -5.396358  -19.3348246427  0.301329
C    -4.38834  -18.8081296427  0.370944
C    -3.08271  -18.1290986427  0.340618
H    -3.100513  -17.0716266427  0.627247
H    -2.523292  -18.5444596427  1.170286
H    -2.485826  -18.3030126427  -0.583809
N    -0.653079  -13.16308  5.929301
C    -0.260037  -13.978599  6.665009
C    0.135124  -15.038157  7.581958
H    0.2406  -14.70189  8.587989
H    -0.524119  -15.884404  7.483578
H    1.130104  -15.329967  7.259074
N    -2.887437  -4.383355  3.860056
C    -3.525556  -4.566651  2.949357
C    -4.429616  -4.737561  1.849352
H    -3.886707  -4.671029  0.909515
H    -4.892929  -5.740036  1.89116
H    -5.214017  -3.987286  1.885568
N    1.596474  -6.153798  6.089263
C    0.779414  -7.002107  6.079813
C    -0.248214  -7.960279  5.959099
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H    -1.084459  -7.463624  5.539114
H    0.015295  -8.661321  5.151874

735



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C    -0.020592  -10.631819  10.717229
C    -1.172596  -9.839223  10.737822
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C    0.637815  -10.97363  11.895062
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C    -0.809805  -9.563403  15.596362
C    2.04292  -11.568518  14.333689
C    2.592436  -12.017024  15.537622
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C    1.016642  -10.716778  16.787973
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H    3.443993  -7.118648  15.939126
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H 1.055052 -7.408872 22.6790890684
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